

Flamprop-isopropyl

Other names:

DL-Alanine, N-benzoyl-N-(3-chloro-4-fluorophenyl)-, 1-methylethyl ester
1-Methylethyl-N-benzoyl-N-(3-chloro-4-fluorophenyl)-dl-alanine
Barnon
Flufenprop-isopropyl
Isopropyl-N-benzoyl-N-(3-chloro-4-fluorophenyl)alanine
Suffix BW
WL 29762

Inchi: InChI=1S/C19H19ClFNO3/c1-12(2)25-19(24)13(3)22(15-9-10-17(21)16(20)11-15)18(23)
InchiKey: IKVXBIIHQGXQRQ-UHFFFAOYSA-N
Formula: C19H19ClFNO3
SMILES: CC(C)OC(=O)C(C)N(C(=O)c1cccc1)c1ccc(F)c(Cl)c1
Mol. weight [g/mol]: 363.81
CAS: 52756-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-149.02	kJ/mol	Joback Method
hf	-497.63	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.466		Crippen Method
mcvol	264.050	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	875.86	K	Joback Method
tc	1104.06	K	Joback Method
tf	536.84	K	Joback Method
vc	0.987	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.32	J/mol×K	875.86	Joback Method
cpg	782.31	J/mol×K	913.89	Joback Method
cpg	794.11	J/mol×K	951.93	Joback Method
cpg	804.78	J/mol×K	989.96	Joback Method
cpg	814.37	J/mol×K	1028.00	Joback Method
cpg	822.97	J/mol×K	1066.03	Joback Method
cpg	830.63	J/mol×K	1104.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52756226&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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